

Efficient Preparation of Quantum States With Exponential Precision

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It has been shown that, starting from the state $|0\rangle$, in the general case, an arbitrary quantum state $|\psi\rangle$ cannot be prepared with exponential precision in polynomial time. However, we show that for the important special case when $|\psi\rangle$ represents discrete values of some real, continuous function $\psi(x)$, efficient preparation is possible by applying the eigenvalue estimation algorithm to a Hamiltonian which has $\psi(x)$ as an eigenstate. We construct the required Hamiltonian explicitly and present an iterative algorithm for removing unwanted superpositions from the output state in order to reach $|\psi\rangle$ within exponential accuracy. The method works under very general conditions and can be used to provide the quantum simulation algorithm with very accurate and general starting states.

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The first step of a quantum algorithm typically consists of resetting all registers to $|0\rangle$ followed by the preparation of an initial state $|\psi\rangle$. In the general case, it has been shown impossible to prepare an arbitrary state with exponential precision in polynomial time [1]. For special cases, however, this is still possible, e.g., when $|\psi\rangle$ represents sampled points of some continuous function $\psi(x)$, and certain integrals over $\psi(x)$ can be evaluated with exponential precision [2]. A useful application of such methods is to prepare initial states for quantum simulation [2].

In this paper we show that quantum states that represent sampled, continuous functions can, under very general conditions, be prepared efficiently. We also provide a method for doing this, using the quantum eigenvalue estimation algorithm by Abrams and Lloyd [3] and the initial state preparation algorithm by Jaksch and Papageorgiou [4].

Suppose that $|\psi\rangle$ represents discrete values of some real function $\psi(x)$. The intuitive idea is that if $|\psi\rangle$ is an eigenvector of the (discretized) Schrödinger equation then it can be obtained by running the eigenvalue estimation algorithm with an initial approximation generated by the technique in [4]. The one-dimensional *continuous* Schrödinger equation for a particle with mass m , in a potential $V(x)$, is defined as

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi(x) = \varepsilon \phi(x), \quad (1)$$

where ε is the energy. For convenience, we will choose units such that $\hbar^2/(2m) = 1$. By defining the potential as

$$V(x) = \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2}, \quad (2)$$

$\psi(x)$ will apparently become an eigenvector with eigenvalue 0. Thus, if 0 is measured from the eigenvalue estimation algorithm we know that the remaining (unmeasured) qubits will be in the state $|\psi\rangle$. More precisely, assume that the continuous Hamiltonian (the expression in brackets in (1)) is discretized into a $2^n \times 2^n$ matrix H , and that $U = e^{iHt}$ can be implemented *exactly* on a quantum computer. An arbitrary eigenvector $|\psi_l\rangle$ of U satisfies

$$e^{iHt} |\psi_l\rangle = e^{i\lambda_l t} |\psi_l\rangle = e^{i2\pi\varphi_l} |\psi_l\rangle. \quad (3)$$

Hence, $\lambda_l t = 2\pi\varphi_l + n2\pi$, with $n \in \mathbb{Z}$ and $\varphi_l \in [0, 1)$. We want to prepare the specific state $|\psi_0\rangle$ for which $\lambda_0 = 0$ (and $\varphi_0 = 0$).

The discrete Hamiltonian H can be written $H = T + V$, where T is the second derivative operator, and V is the potential. The norm of the former is $\|T\| = 2^{2n}$ [5]. We make the assumption that $\|V\| = O(2^{2n})$, so that $\|H\| \leq \|T\| + \|V\| \leq 2^{2n+p}$ for some integer p , independent of n . For simplicity, we also assume that all elements of V are positive [8], making H positively semidefinite, and that $\min_{l \neq 0} \lambda_l = O(1)$, independent of n . By choosing $t = 1/2^{2n+p}$ all eigenvalues of U will apparently fall in the first quadrant, i.e., $\varphi_l < 1/4$ for all l .

Now, suppose that the eigenvalue estimation algorithm is started in the state

$$|0\rangle |\Psi_0\rangle = \sum_{l=0}^{2^n-1} d_l |0\rangle |\psi_l\rangle, \quad (4)$$

where the first register consists of only a single qubit. At the final step of the algorithm, before measurement, the state will be

$$\sum_{l=0}^{2^n-1} d_l (g(\varphi_l, 0)|0\rangle + g(\varphi_l, 1)|1\rangle) |\psi_l\rangle. \quad (5)$$

Here, the function g is defined as (see [4])

$$g(\varphi_l, j) = \begin{cases} \frac{\sin(\pi(2\varphi_l - j))e^{\pi i(\varphi_l - j/2)}}{2\sin(\pi(\varphi_l - j/2))}, & 2\varphi_l \neq j \\ 1, & 2\varphi_l = j. \end{cases} \quad (6)$$

We remark that for the case $j = 0$, $\varphi_l \neq 0$, g reduces to $g(\varphi_l, j) = \cos(\pi\varphi_l)e^{i\pi\varphi_l}$. The probability of measuring the first qubit in the state $|0\rangle$, ensuring that $|\psi_0\rangle$ is still in the superposition, is

$$P_1 = \sum_{l=0}^{2^n-1} |d_l|^2 |g(\varphi_l, 0)|^2. \quad (7)$$

Assuming that 0 is measured, the second register will collapse to

$$|\Psi_1\rangle = \frac{1}{\sqrt{P_1}} \sum_{l=0}^{2^n-1} d_l g(\varphi_l, 0) |\psi_l\rangle. \quad (8)$$

From induction it follows that repeated use of this procedure leads to

$$P_k = \frac{1}{P_1 \cdots P_{k-1}} \sum_{l=0}^{2^n-1} |d_l|^2 |g(\varphi_l, 0)|^{2k} \quad (9)$$

$$|\Psi_k\rangle = \frac{1}{\sqrt{P_1 \cdots P_k}} \sum_{l=0}^{2^n-1} d_l (g(\varphi_l, 0))^k |\psi_l\rangle. \quad (10)$$

The probability of measuring 0 every time (probability of success) is therefore

$$P_1 \cdots P_k = \sum_{l=0}^{2^n-1} |d_l|^2 |g(\varphi_l, 0)|^{2k} \geq |d_0|^2 |g(\varphi_0, 0)|^{2k} = |d_0|^{2k}. \quad (11)$$

The last equality follows since $\varphi_0 = 0$. With the method for initial state preparation in [4] we can make $|d_0|^2 > 1/2$. From the expression for $|\Psi_k\rangle$ it is clear that only states with $|g(\varphi_l, 0)|$ close to 1 ($\varphi_l \leq 1/\sqrt{k}$) will survive as k grows. If we choose, e.g., $k = 2n$ all states with $\varphi_l \geq 1/4$ will have their amplitudes decreased by a factor more than $1/2^{2n}$. By choosing a new value of t , $t' = 2t$ we can reduce a second set of amplitudes exponentially. After $2n + p$ such steps we are left with

$$P_k^{(2n+p)} = \frac{1}{P_1^{(0)} \cdots P_k^{(0)} \cdots P_1^{(2n+p)} \cdots P_{k-1}^{(2n+p)}} \sum_{l=0}^{2^n-1} |d_l|^2 |g(\varphi_l, 0) \cdots g(2^{2n+p}\varphi_l, 0)|^{2k} \quad (12)$$

$$|\Psi_k^{(2n+p)}\rangle = \frac{1}{\sqrt{P_1^{(0)} \cdots P_k^{(0)} \cdots P_1^{(2n+p)} \cdots P_k^{(2n+p)}}} \sum_{l=0}^{2^n-1} d_l (g(\varphi_l, 0) \cdots g(2^{2n+p}\varphi_l, 0))^k |\psi_l\rangle \quad (13)$$

$$P(\text{success}) = \sum_{l=0}^{2^n-1} |d_l|^2 |g(\varphi_l, 0) \cdots g(2^{2n+p}\varphi_l, 0)|^{2k} \geq |d_0|^2 |g(\varphi_0, 0) \cdots g(2^{2n+p}\varphi_0, 0)|^{2k} = |d_0|^{2k}. \quad (14)$$

The condition that $\min_{l \neq 0} \lambda_l = O(1)$ ensures that at least one of the terms $g(2^j \varphi_l, 0)$ will satisfy $g(2^j \varphi_l, 0) \leq 1/A$, for some $A > 1$, independent of n and k . Hence, if k is polynomial in n the only term in the superposition that is not exponentially reduced is $|\psi_0\rangle$. The algorithm can be implemented as a sequence of $(2n + p)k$ circuits of the type in Fig. 1, where $U^{(s)} = \exp(iH2^s t)$.

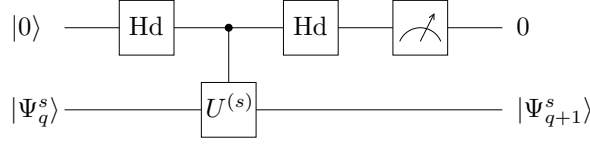


FIG. 1: Schematic description of one step of the quantum state preparation algorithm. Here, Hd means the Hadamard gate; $U^{(s)} = \exp(iH2^s t)$. When q reaches some value k it is reset to 0 and s is increased with 1.

The requirement that U can be implemented exactly can be weakened to requiring only exponential precision. In Fig. 1 the state before measurement is

$$\frac{1}{2}|0\rangle(I + U^{(s)})|\Psi_q^{(s)}\rangle + \frac{1}{2}|1\rangle(I - U^{(s)})|\Psi_q^{(s)}\rangle. \quad (15)$$

The probability of measuring 0 is $P_q^{(s)} = \|I + U^{(s)}\|^2/4$. For this outcome the second register will collapse to

$$\frac{1}{2\sqrt{P_q^{(s)}}}(I + U^{(s)})|\Psi_q^{(s)}\rangle. \quad (16)$$

Suppose now that $\tilde{U}^{(s)} = U^{(s)} + \Delta$ can be implemented with exponential precision, i.e., $\|\Delta\| = O(1/2^n)$. For this case, we derive a lower bound on the probability of success. First, we make the following observation:

$$\begin{aligned} \left| \sqrt{\tilde{P}_q^{(s)}} - \sqrt{P_q^{(s)}} \right| &= \frac{1}{2} \left| \|(I + \tilde{U}^{(s)})|\Psi_q^{(s)}\rangle\| - \|(I + U^{(s)})|\Psi_q^{(s)}\rangle\| \right| \\ &\leq \frac{1}{2} \|(U^{(s)} - \tilde{U}^{(s)})|\Psi_q^{(s)}\rangle\| = \frac{1}{2} \|\Delta|\Psi_q^{(s)}\rangle\| \leq \frac{\|\Delta\|}{2}. \end{aligned} \quad (17)$$

From (17) it follows directly that $|\tilde{P}_q^{(s)} - P_q^{(s)}| < \|\Delta\|$. Using this result we get

$$\tilde{P}_1^{(0)} \dots \tilde{P}_k^{(2n+p)} \geq (P_1^{(0)} - \|\Delta\|) \dots (P_k^{(2n+p)} - \|\Delta\|) = P_1^{(0)} \dots P_k^{(2n+p)} (1 - O(\|\Delta\|))^{k(2n+p)}, \quad (18)$$

which is bounded by a constant for exponentially small $\|\Delta\|$ [9]. Using (17) and the definition of $P_q^{(s)}$ we may also derive an upper bound on the difference between $|\tilde{\Psi}_{q+1}^{(s)}\rangle$ and $|\Psi_{q+1}^{(s)}\rangle$

$$\begin{aligned} \||\tilde{\Psi}_{q+1}^{(s)}\rangle - |\Psi_{q+1}^{(s)}\rangle\| &= \frac{1}{2} \left\| \frac{1}{\sqrt{\tilde{P}_q^{(s)}}}(I + U^{(s)} + \Delta)|\Psi_q^{(s)}\rangle - \frac{1}{\sqrt{P_q^{(s)}}}(I + U^{(s)})|\Psi_q^{(s)}\rangle \right\| \\ &\leq \frac{\left| \sqrt{\tilde{P}_q^{(s)}} - \sqrt{P_q^{(s)}} \right|}{\sqrt{\tilde{P}_q^{(s)}}} + \frac{1}{2\sqrt{\tilde{P}_q^{(s)}}}\|\Delta\| \leq \frac{\|\Delta\|}{\sqrt{\tilde{P}_q^{(s)}}} = O(\|\Delta\|). \end{aligned} \quad (19)$$

It can be shown [6] that the total error of the algorithm is at most the sum of the errors of the individual blocks. Hence, with the previous choice of k ,

$$\|\Delta_{\text{tot}}\| \leq (2n + p)kO(\|\Delta\|) = O(n^2/2^n). \quad (20)$$

We now consider the implementation of U . Suppose that we use an m :th order splitting formula (see [7]) to approximate $U^{(s)}$:

$$U^{(s)} = e^{iH2^s t} = \prod_{j=1}^m e^{i w_j G_j 2^s t} - \Delta, \quad (21)$$

where w_j are weight factors and G_j is either T or V . Defining the product on the right hand side $\tilde{U}^{(s)}$ it follows from the definition of the matrix exponential that Δ is the Taylor expansion of $\tilde{U}^{(s)} - U^{(s)}$ beyond m :th order. Provided

that $V(x)$ can be efficiently computed to exponential precision on a classical computer, both e^{iVt} and e^{iTt} can be efficiently calculated on a quantum computer, as described in [2].

The norm of Δ is of order $O((2^st)^m(\|T\| + \|V\|)^m)$. For some $B_* \geq 1$ we impose the (not very restrictive) condition $\|T\|_* + \|V\|_* \leq B_*\lambda_*$, where the norm is defined on a subspace spanned by a number of basis vectors $|\psi_l\rangle$ of H , containing not only the ground state, and λ_* is the maximum eigenvalue of these vectors [10]. Defining $B = \sup B_*$, where the supremum is taken over all subspaces, we choose t as $t = 1/(B2^{n+p})$. For $k = -\lceil n/\log_2(\pi/(4B)) \rceil$ all states with $\varphi_l > 1/(4B)$ will have their amplitudes decreased by a factor more than $1/2^n$.

We are now in position to modify the previous error analysis. If $2^{st}B\lambda_* \leq 1/C$, for some $C > 1$ independent of m , the error in (21) will be exponentially small, of order $O(1/C^m)$, on the subspace where λ_* is defined.

$$\begin{aligned} \left| \sqrt{\tilde{P}_q^{(s)}} - \sqrt{P_q^{(s)}} \right| &\leq \frac{1}{2} \|\Delta|\Psi_q^{(s)}\rangle\| \leq \frac{1}{2|d_0|} \left\| \Delta \sum_{l=0}^{2^n-1} d_l(g(\varphi_l, 0) \cdots g(2^s\varphi_l, 0))^q |\psi_l\rangle \right\| \\ &\leq O\left(\frac{1}{C^m}\right) + \frac{\sqrt{2}}{2} \|\Delta\| \left\| \sum_{2^{st}B\lambda_l \geq 1} d_l(g(\varphi_l, 0) \cdots g(2^s\varphi_l, 0))^k |\psi_l\rangle \right\|. \end{aligned} \quad (22)$$

For the eigenvectors in the sum in (22), if $2^{st}\lambda_l \geq 2\pi$, then at least one of the arguments $2^j\varphi_l$ will be $O(1)$, and, hence, the amplitude of this state will be exponentially reduced. If $2^{st}\lambda_l < 2\pi$, on the other hand, then $2^s\varphi_l \geq 1/(2\pi B)$. We make the assumption that B is bounded from above by a polynomial in n . Hence,

$$\left| \sqrt{\tilde{P}_q^{(s)}} - \sqrt{P_q^{(s)}} \right| = O\left(\frac{1}{C^m}\right) + O(1)O\left(\frac{1}{D^k}\right), \quad (23)$$

where D is greater than 1 independent of k . The fact that $\|\Delta\| = O(1)$ follows since $\|U^{(s)}\| = \|\tilde{U}^{(s)}\| = 1$. By choosing k as above, and m polynomial in n the right hand side of (23) can be made exponentially small in n . In the same way it is possible to prove that $\|\tilde{\Psi}_k^{(s)} - |\Psi_k^{(s)}\rangle\|$ will also be exponentially small in n , and, thus, the same holds for the total error. In practice, one would have to guess the value of B . However, as long as the guessed value is larger than the true B it does not have to be very accurate.

For the sake of clarity, we have not yet discussed the issue of boundary conditions, but rather assumed implicitly that $\psi(0) = \psi(1) = 0$. This will be the case for most problems of practical interest and is also a requirement for the method in [4] to work. Here, however, we will briefly outline a scheme for generalizing our method to functions with non-zero boundary conditions. One way of doing this is to extend the function to be prepared by smoothly attaching exponentially decaying tails on both sides. Practically, this can be achieved by adding, say, two extra qubits to the register holding the function to be prepared. As an example, states starting with qubits 00 will represent the left hand side tail; states starting with qubits 01 will represent the original function ψ ; and states starting with qubits 10 and 11 will represent the right hand side tail. At the end of the preparation we will be left with the extended function. To get rid of the tails we can now measure the two qubits that we added to the register. With high probability this measurement will yield 01, implying that the extended state has collapsed to the original function ψ .

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- [9] In fact, this is true even for polynomially small $\|\Delta\|$.
- [10] The inequality $\|T\| + \|V\| \leq \|H\| + 2\|V\|$ is trivial. Suppose that ψ is some eigenvector of H with eigenvalue λ . For the case $V > \lambda$, ψ decays exponentially as $e^{\lambda-V}$. Hence, if λ is the maximum eigenvalue on some subspace spanned by eigenvectors of H , the norm $\|V\|$ will normally be of order λ . The right hand side of the inequality will then also be of order λ on this subspace.